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A GRAPH THEORETICAL AND TOPOLOGICAL APPROACH TO CHEMICAL STRUCTURE, REACTIVITY AND DYNAMICS

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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

This report summarizes work done by the mathematical chemistry group at the University of Georgia during the period 1984-1988 on applications of graph theory, topology, and group theory to problems in the areas of chemical structure, chemical reactivity, and chemical dynamics. Applications of these theoretical methods to superconductivity, surface science, fuel design, medicine, and environmental technology have been identified. A list of 108 publications arising from this project has been appended.

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The funding provided by the Office of Naval Research under the SRO4 program has allowed a research group in mathematical chemistry to be established at the University of Georgia. The general objective of this group has been the discovery and development of new applications of mathematical disciplines, particularly graph theory and topology, to various areas of chemical interest including chemical structure, reactivity, and dynamics. Dr. R. Bruce King, Regents' Professor of Chemistry, has been responsible for the overall direction of this group and for the portions of the research concerned with applications of graph theory and topology for the study of metal clusters and superconductors. Dr. Dennis H. Rouvray, Associate Research Scientist, has been responsible for the development of topological indices and other graph invariants for the study of structure-property relationships. Dr. M. Howard Lee, Professor of Physics, has been responsible for the development of the method of recurrence relations to studies of properties of metals, metal clusters, and other physical systems of interest. Dr. E. Rodney Canfield, Professor of Computer Science, has been responsible for mathematical and computational aspects of this project with particular emphasis on relevant areas of algorithm development. The research contributions to mathematical chemistry of two of these senior investigators, namely Dr. King and Dr. Rouvray, have been recognized by the University of Georgia through awards of Creative Research Medals in 1985 and 1988, respectively.

This project has been very productive since 82 publications have already appeared from this work with an additional 12 publications in press and an additional 14 manuscripts submitted for publication (see attached publication lists). In addition, results from this project have been presented at 36 different scientific meetings during the past four years (see attached list). Such presentations have included papers describing new mathematical methods relevant to chemical problems as well as new applications of such methods. In addition, the mathematical chemistry group

organized a major conference, namely a conference on "Graph Theory and Topology in Chemistry," which was held at the University of Georgia during the period March 15-20, 1987. This conference attracted approximately 70 participants, including participants from Great Britain, Canada, Yugoslavia, Bulgaria, Japan, China, and Mexico. The program of the conference included approximately 45 oral presentations, which were published by Elsevier Scientific Publishing Company in a Conference Volume edited by R.B. King and D.H. Rouvray (publication 54 on the attached list).

Another important activity of the mathematical chemistry group at the University of Georgia has been the founding of the new Journal of Mathematical Chemistry published by Balzer Verlag of Switzerland and edited by Dr. Rouvray. Publication of this journal began in January, 1987, and the journal was officially launched at our international conference mentioned above. Under the editorship of Dr. Rouvray the journal has so far received a warm welcome and continues to grow in support, both in terms of the number of papers being submitted and the number of subscriptions being taken out. At the present time, the journal appears four times per year.

An important result of the research has been the identification of a number of applications of chemical topology, chemical graph theory, and related disciplines to areas of practical interest, such as superconductivity, surface science, fuel design, medicine, and environmental technology. Research proposals relating to some of these applications have been submitted to seek funding for support of key portions of the mathematical chemistry group past the termination of the ONR SRO4 project. Currently pending is a proposal to the Office of Naval Research, relating to superconductivity and metal clusters, as well as a proposal to the Air Force Office of Scientific Research, relating to fuel design.

RESEARCH RESULTS

Highlights of our research during the four-year project period are summarized below according to senior investigators (King, Rouvray, Lee, and Canfield). Publication citations refer to numbers on the attached publication lists.

R.B. King:

Professor King's major contributions to this project have been in the following areas:

a. The Topology of Superconductors: An important achievement during this research project has been the development of a novel topological approach to the chemical bonding in superconductors, which is applicable to the new high-temperature copper oxide superconductors as well as more established classes of superconductors.[37,38,44,56,62,93] An important conclusion from this work is that the maximum T_c obtainable from layered copper oxide structures will be no higher than 180 K and that a further major breakthrough, comparable to the original discovery of the high-temperature copper oxide superconductors by Bednorz and Müller, will be needed before room-temperature superconductivity is achieved.[93] This observation suggests the importance of further fundamental research on superconductivity including the structures of and chemical bonding in superconductors in addition to applied research on fabrication of the existing types of copper oxide superconductors.

b. Metal Cluster Topology: During the course of this project, Professor King developed topological and graph-theoretical approaches to the chemical bonding in osmium,[15] gold,[7,16] platinum,[7,17] rhodium,[18,20] and cobalt[59] clusters, including prototypical examples of metal clusters exhibiting such interesting features as fused polyhedra (rhodium carbonyl clusters), stacked triangles with Möbius bonding at each end of the stack (platinum carbonyl clusters), non-

spherical bonding manifolds of vertex atoms (gold clusters), and interstitial carbon atoms (cobalt carbonyl clusters). Professor King also extended his graph-theory derived treatment of metal cluster bonding topology to metal carbonyl clusters with alkylphosphinidene vertices [94] and to mercury vertices in transition metal clusters and metal amalgam clusters.[65] He has also made a detailed study of the chemical bonding topologies in six-vertex metal clusters, as well as their polyhedral rearrangements.[66] This last work makes use of Gale diagrams, the chemical applications of which have been developed further by Professor King during the course of this research project.[28,85] Professor King has also shown that the graph-theory derived approach to metal cluster bonding can be extended to infinite one-dimensional and two-dimensional early transition metal and lanthanide structures leading to reasonable results relating to heats of atomization and alloy systematics in the limiting case of bulk metal structures.[34] This work is significant in connection with the application of graph-theory derived methods to the study of the properties of solid state materials, including the superconductors discussed above. In addition, Professor King has shown that elementary chemical bonding ideas, coupled with principles from solid state physics not unrelated to his approach to metal cluster bonding topology, can account for the shapes of the rectangular and hexagonal lattices found in islands of silver and gold atoms deposited on the surface of highly oriented pyrolytic graphite as determined by scanning tunneling microscopy under atomic resolution.[67] This work is significant in connection with the application of topological methods to the study of the properties of surfaces with potential applications in heterogeneous catalysis and related areas. Professor King's theoretical ideas on metal cluster chemical bonding have suggested some novel gas phase post-transition metal cluster experiments which have been performed

by Professor Michael Duncan of the University of Georgia. Initial results from this experimental work have demonstrated for the first time the close connection between post-transition metal clusters in the gas and condensed phases[35,58] and have led to the identification of a number of novel homometallic and heterometallic gas phase clusters containing metals such as tin, lead, antimony, and bismuth.[29,68,69]

c. Topology of Polyhedral Boranes: Professor King has made extensive use of graph-theory derived methods for the study of the chemical bonding topology of metal clusters. An important question is the relationship of such qualitative methods to various computational approaches. In this connection, Professor King has examined topological aspects of computations of orbital energies of the deltahedral boranes, which are much simpler to study than metal clusters because of the absence of d orbitals. Professor King's initial work in this area involved an examination of the relationship between graph-theory derived and extended Hückel approaches to the chemical bonding in octahedral and icosahedral boranes.[30] Subsequently, he extended this study to the analysis of more advanced self-consistent molecular orbital computations and to deltahedra other than the most regular deltahedra.[61] Professor King has now initiated a collaboration with Professor Benjamin Gimarc of the University of South Carolina where Professor Gimarc's group provides more detailed information on the computed molecular orbital energies of all of the deltahedral borane anions $B_nH_n^{2-}$ and related molecules for comparison with the predictions from graph-theoretical and topological methods.

d. Polyhedral Topology: During the course of this project, Professor King made detailed studies of isomerizations in seven[2] and eight[5] vertex polyhedra. Each time a vertex is added to the polyhedron under consideration, new mathematical

methods need to be developed because of the exponentially increasing number of possible polyhedra. Professor King also wrote an invited review article on polyhedral isomerizations for publication in Volume 2 of "Advances in Dynamic Stereochemistry."[28]

e. Symmetry and Chirality: During the course of this project, Professor King has made major progress in the area of chirality algebra. In this connection, he has made a detailed study of chirality in transitive skeletons having six or less sites. This has involved a generalization of the concept of chirality to permutation groups not corresponding to three-dimensional symmetry point groups in order to provide a more detailed understanding of such topics as qualitatively complete chirality functions.[26] In addition, Professor King has recognized some special features of the chiral ligand partitions of regular polyhedra which have allowed him to calculate for the first time the lowest degree chirality polynomial of the regular icosahedron, a problem previously assumed to be intractable.[27] Professor King has also expanded, extended, and corrected some preliminary 1976 results of the Soviet scientist, V.I. Sokolov. This work has led to a simpler, but nevertheless useful approach for the study of chirality in chemically significant polyhedra.[70] Professor King has also written a detailed review which summarizes the use of chirality algebra to determine polynomials for the description of chirality observations.[60] This review presents a critical analysis of the limitations of such mathematical methods.

f. Differential Equations: Professor King has examined two very diverse approaches for the study of differential equations of potential chemical and physical significance, namely Painlevé analysis and kinetic logic. He has developed a new simplified approach for the classification of higher order integrable differential equations according to their Painlevé properties, leading to the novel

concept of Painlevé chains.[14,36] Professor King has also investigated applications of kinetic logic[71,74] for the study of immunological control networks.[55,57] These ideas are closely related to the kinetic logical method for the study of dynamic systems, but require major modifications of earlier approaches because of the specific properties of the variables describing immunological control networks.

D. H. Rouvray:

Dr. Rouvray's major contributions to the project have involved the modeling of chemical systems using topological methods, particularly those based on graph theory. Some highlights of this work are summarized below.

a. Wiener Topological Index and Tree Graphs: In 1985 Canfield, Robinson, and Rouvray published a paper demonstrating for the first time how the Wiener topological index can be calculated for any tree graph.[4] This paper not only showed how the Wiener index could be relatively simply calculated for very complex structures, but also led to renewed interest in this index worldwide. This interest has resulted in further development of the ideas initiated in this paper, the writing of computer programs for the indices, and the first demonstration by Bonchev and collaborators of the close relationship of this index to quantum mechanical parameters. We are thus now on the verge of understanding why topological indices work so well in many different chemical settings.

b. Relationship of Topological Indices to Fractals: In 1986 Rouvray and Pandey published a paper which proved for the first time the close connection between the fractal nature of alkane molecules and their topological indices.[22] Fractals are ubiquitous in nature and our work demonstrated that fractal concepts apply in the molecular domain as well. The precise nature of the relationship was

elucidated by applying scaling theory to correlations of the Wiener index against various physicochemical properties of alkane systems. It was shown how it was possible to obtain fractal dimensionalities for individual species through their topological indices and thereby to gain valuable insight into their geometrical conformation. This approach is quite general and can be readily extended to any chain-like species, including branched molecules.

c. Topological Aspects of Soot Formation in Hydrocarbons: In 1987 Hanson and Rouvray published a paper dealing with the formation of soot in hydrocarbon fuel molecules.[40] The parameter we studied was the threshold soot index and we investigated this for a number of fuel mixtures. We were able to demonstrate for the first time that the soot threshold index can be correlated with a composite topological index that we developed. Even though many of the data points used in our correlation were unreliable, we were able to obtain an overall correlation coefficient of 0.974. This work has stimulated new approaches to the study of fuel molecules based on topological modeling of these species.

d. Molecular Connectivity and Absorption Spectra: In 1988 Rouvray and El-Basil published a paper showing for the first time the intimate connection of absorption spectra in polycyclic aromatic hydrocarbons with the Randic' molecular connectivity index.[83] Excellent correlations were obtained for both the beta and para electronic absorption bands. Moreover, we employed for the first time a new data reduction technique. Instead of calculating topological indices for the full graphs of these hydrocarbons, we first reduced them to their caterpillar trees and then calculated the indices for the trees. To our great surprise, the correlations based on the derived tree structures were better than those obtained on the original graphs. This discovery opens the way for calculations based on large and complex molecules.

M.H. Lee

Professor Lee's major contributions to this project have involved applications of the method of recurrence relations to studies of topological and graph-theoretical properties of metals, metal clusters, and other physical systems of interest as well as further development of the underlying mathematics of the recurrence relation method. Important achievements of Professor Lee's research during the course of this project include the following:

a. Exact Dynamically Convergent Calculations of the Dynamic Structure Factor of Metals: Dynamic properties of liquids and solids are obtained experimentally by neutron and x-ray scattering measurements. Hong and Lee[9] have shown how the structure factor can be calculated from first principles analytically or numerically, but without parametrization. The theoretical structure factor compares favorably with the experimental.

b. Acoustical and Optical Properties of Solids: Linearly coupled harmonic oscillators have been the basic models for acoustic and optical properties of solids. Florencio and Lee have obtained the dispersion relation, energy spectrum, and propagation of such systems.[12]

c. Electronic Properties of a Two-Dimensional System: Most present electronic devices are built using semiconductor materials. A key feature of these devices is their quasi two-dimensional character. Lee and Hong have shown how the method of recurrence relations can be used to obtain complete time evolution solutions for electron density fluctuations at long wavelengths.[10]

d. Kimball's Formula: Kimball's formula relates the pair correlation function at the origin to the structure factor at an infinity. This formula has been generally believed to be exact. We have now found that this formula breaks down at high densities.[13,73] Considerable care must thus be exercised in the use of Kimball's

formula to simplify many-body calculations.

e. Dimension Dependence of the Susceptibility of a Free Electron Gas: The free electron gas is a widely used model for static properties of metals. The susceptibility is a response function which describes the response of a charged system to an external probe. Sharma and Lee have obtained an exact expression for the susceptibility at any dimension, integer or noninteger.[19] Fractional dimensions are now important for fractal analysis of nonuniform geometries.

f. Dynamic Equivalence: The method of recurrence relations shows that dynamic equivalence between two dissimilar systems is possible if they have common dynamic parameters. Dynamic parameters consist only of the dimensionality and hypersurface of a realized Hilbert space. This equivalence notion has let us to discover that the time evolution in the two-dimensional quantum electron gas is the same as that in the classical one-dimensional harmonic oscillator chain with an impurity.[X6] This new idea opens up a vast area of time evolution problems for recurrence relation analysis.

g. Classical Problems: The method of recurrence relations has been further extended so as to be applicable to classical problems. This extension has allowed us to obtain the time evolution in such classical systems as diatomic chains of harmonic oscillators, classical fluids, abnormal electron fluids (a possible model for high T_c superconductivity), and electron beam propagation in inhomogeneous media (e.g., the atmosphere).[89,90]

h. Further Development of the Recurrence Relation Method: We find that the method of recurrence relations rests on a deep mathematical foundation initially suggested by several successful physical applications. In particular, the Bessel equality provides an essential link between Hilbert space theory and nonequilibrium statistical mechanics and has led to a new way of obtaining an

analytic theory of continued fractions and ratios of infinite products, including the remarkable formula due to Wallis.[75,91,92]

E.R. Canfield:

Professor Canfield's major contributions to this project have been in the following areas:

a. Maps of Surfaces: Such maps are generalizations of the convex polyhedra so common in chemical applications. During the last twenty years, Tutte and others have developed an extensive theory for the planar case. However, maps on surfaces of larger genus have been for the most part unexplored territory. We have developed generating functions for arbitrary genus and have analyzed the coefficients asymptotically.[46,80,81,X2] This work, along with results obtained by Wormald and Bender's student Gao, have suggested an underlying structure which is not yet properly explained. Thus, this work is continuing and being pursued by several other researchers at the present time. It is this part of Professor Canfield's work which forms part of a research proposal recently funded by the National Security Agency.

b. Planarity: There are two widely known algorithms for planarity testing, both of which are linear in complexity. In work with S.G. Williamson, we have shown a surprising and totally unexpected connection which reveals that in a certain sense these two algorithms are in fact the same. This work also resulted in an improved exposition of one of the algorithms. Professor Williamson has used this work as the starting point for a new research proposal to make comparative studies of other practical and economically important algorithms.

c. Sparse Graphs: Sparse graphs are graphs with n vertices whose edge counts are nowhere near the quadratic upper limit, but rather are of the form xn where x is either constant or a slowly growing function of n. Most graphs with physical

applications are of this nature. Work with Bender and McKay suggests a very interesting counting formula for these graphs. This formula and its proof should have some interesting connections with other research. The proof is still incomplete at the moment, although the prospects for completing the proof appear promising.

d. Nonradical Algebraic Numbers: Considerable amounts of nineteen century mathematics, virtually ignored in modern times, may be useful in physical applications in the treatment of nonlinear systems described by evolution equations. Works by Klein, Hermite, Kiepert, Kronecker, and others on solutions of quintic equations with elliptic functions suggest many interesting features of the later class. We have written several manuscripts gathering this material together in a readable manner. We have formulated an entire algorithm for solving the quintic equation, probably the first time such an algorithm has been written out thoroughly in one place.[X14] This algorithm has been successfully tested by implementing a working computer program. We have a useful library of routines, including the arithmetic/geometric mean algorithm, for carrying out numerical experiments on these special functions. This work has also involved some study of classical invariant theory.

e. Software Development: A Pascal preprocessor has been developed by Mr. Latif Khalil as part of his M.A.M.S. work and during an extra summer of consulting. This software in effect extends the Pascal language to include new data types such as large integers, rational numbers, complex numbers, polynomials, etc., which the user defines once and for all in a library. New software has also been developed for the computation of various topological indices for Dr. Rouvray's work, as well as for various calculations related to elliptic functions for the work on nonradical algebraic numbers discussed above.

SCIENTIFIC PUBLICATIONS ISSUED AS TECHNICAL REPORTS

The 94 publications listed below have been issued as technical reports during the project period. Their numbers on the list below correspond to their technical report numbers.

1. King, R.B.; Rouvray, D.H. "Isomer Enumeration in Polytertiary Phosphines and Related Compounds," Phosphorus and Sulfur, 1985, 22, 177-182.

2. King, R.B. "Chemical Applications of Topology and Group Theory. 18. Polyhedral Isomerizations of Seven-Coordinate Complexes," Inorg. Chem., 1985, 24, 1716-1719.

3. King, R.B. "Chemical Applications of Topology and Group Theory. 17. An Information Theoretical Approach to Polyhedral Symmetry," Theor. Chim. Acta, 1985, 68, 143-153.

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6. King, R.B.; Rouvray, D.H., "Chemical Application of Topology and Group Theory. 19. The Even Permutations of the Ligands in Five-Coordinate Complexes Viewed as Proper Rotations of the Regular Icosahedron," Theor. Chim. Acta, 1986, 69, 1-10.

7. King, R.B. "Metal Cluster Topology: Applications to Gold and Platinum Clusters," in "Mathematics and Computational Concepts in Chemistry," (Ed., N. Trinajstic), Ellis Horwood Ltd., Chichester, 1986, pp. 146-154.

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10. Lee, M.H.; Hong, J. "Time and Frequency Dependent Behavior of a Two-Dimensional Electron Gas at Long Wavelengths," Phys. Rev. B, 1985, 32, 7734-7742.

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15. King, R.B. "Metal Cluster Topology. 1. Osmium Carbonyl Clusters," Inorg. Chim. Acta, 1986, 116, 99-107.

16. King, R.B. "Metal Cluster Topology. 2. Gold Clusters," Inorg. Chim. Acta, 1986, 116, 109-117.

17. King, R.B. "Metal Cluster Topology. 3. Platinum Carbonyl Clusters," Inorg. Chim. Acta, 1986, 116, 119-124.

18. King, R.B. "Metal Cluster Topology. 4. Rhodium Carbonyl Clusters Having Fused Polyhedra," Inorg. Chim. Acta, 1986, 116, 125-133.

19. Sharma, N.L.; Lee, M.H. "Wave Vector Dependent Susceptibility of a Free Electron Gas in D Dimensions and the Singularity at $2k_F$," J. Math. Phys., 1986, 27, 1618-1628.

20. King, R.B. "Graph Theory in the Study of Metal Cluster Bonding Topology: Applications to Metal Clusters Having Fused Polyhedra," Int. J. Quant. Chem., 1986, S20, 227-238.

21. Rouvray, D.H. "The Prediction of Biological Activity Using Molecular Connectivity Indices," Acta Pharm. Jug., 1986, 36, 239-252.

22. Rouvray, D.H.; Pandey, R.B. "The Fractal Nature, Graph Invariants, and Physicochemical Properties of Normal Alkanes," J. Chem. Phys., 1986, 85, 2286-2290.

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67. King, R.B. "Chemical Bonding in Two-Dimensional Islands of Silver and Gold on Graphite Surfaces," Chem. Phys. Lett., 1988, 149, 562-564.

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87. Rouvray, D.H. "The Limits of Applicability of Topological Indices," J. Mol. Struct. THEOCHEM, in press.

88. Rouvray, D.H. "The Pioneering Contributions of Cayley and Sylvester to the Mathematical Description of Chemical Structure," J. Mol. Struct. THEOCHEM, in press.

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94. King, R.B. "Metal Cluster Topology. 7. Metal Carbonyl Clusters with Alkylphosphinidene Vertices, " New J. Chem., in press.

SCIENTIFIC PUBLICATIONS FROM THE ONR PROJECT NOT YET ISSUED AS TECHNICAL REPORTS

X1. Gutman, I.; Rouvray, D.H. "Mathematical Characteristics of the Wiener Molecular Branching Index," submitted for publication (Chem. Phys. Lett.).

X2. Bender, E.A.; Canfield, R.R.; Robinson, R.W. "The Asymptotic Number of Tree-Rooted Maps on a Surface," J. Comb. Theory, A, in press.

X3. Canfield, E.R. "Menage Numbers, Bijections, and P-Recursiveness," Discrete Mathematics, 1987, 63, 117-129.

X4. Canfield, E.R.; Williamson, S.G. "A Combinatorial Study of Straightening Bases," J. Lin. Multilin. Algebra, in press.

X5. Lee, M.H. "Frequent Moment Sum Rules, Recurrence Relations, and Continued Fractions in Nonequilibrium Statistical Mechanics," submitted for publication (J. Computer Phys. Commun.).

X6. Lee, M.H.; Florencio, J.; Hong, J. "Dynamic Equivalence of a Two-Dimensional Electron Gas and a Classical Harmonic Oscillator Chain with an Impurity," submitted for publication (Phys. Rev. Lett.).

X7. *Canfield, E.R.; Williamson, S.G. "The Two Basic Linear Time Planarity Algorithms:* Are They the Same?," submitted for publication (J. Lin. Multilin. Algebra).

X8. Rouvray, D.H. "The Evolution of the Concept of Molecular Similarity," in "Computer-Based Methods of Molecular Similarity," (Eds., G. Maggiora and M.A. Johnson), Wiley and Sons, in press.

X9. Rouvray, D.H. "The Chemical Applications of Combinatorics," in "Handbook of Combinatorics," (Eds., M. Grötschel, R.L. Graham, and L. Lovász), North Holland Publishing Company, in press.

X10. Randić, M.; El-Basil, S. "Graph-Theoretical Analysis of Large Benzenoid Systems," submitted for publication (J. Math. Chem.).

X11. El-Basil, S.; Randić, M. "On Clar Valence Structures on Non-Branched Benzenoid Hydrocarbons," submitted for publication (Int. J. Quant. Chem.).

X12. El-Basil, S. "Fibonacci Numbers in the Topological Theory of Benzenoid Hydrocarbons and Related Graphs," submitted for publication (J. Math. Chem.).

X13. King, R.B. "The Group-Theoretical Structure of Algebraic Equations. 1. Non-Radical Algebraic Numbers as Theta Functions," submitted for publication (SIAM Journal on Algebraic and Discrete Methods).

X14. King, R.B.; Canfield, E.R. "The Group-Theoretical Structure of Algebraic Equations. 2. Roots of the General Quintic Equation as Illustrations of the Least Complicated Examples of Non-Radical Algebraic Numbers," submitted for publication (SIAM Journal on Algebraic and Discrete Methods).

CUMULATIVE LIST OF PAPERS BASED ON ONR WORK PRESENTED AT SCIENTIFIC MEETINGS

1. Conference on Combinatorics of Ordered Sets, Mathematical Forschungsinstitut Oberwolfach, West Germany, January 27 - February 2, 1985:
   E.R. Canfield, "Ménage Numbers, Bijections, and P-Recursiveness."

2. Sixteenth Southeastern International Conference on Combinatorics, Graph Theory, and Computing, Florida Atlantic University, Boca Raton, Florida, February 11-15, 1985:
   D.H. Rouvray, "Topological Indices as Chemical Behavior Descriptors."

3. Spring Topology Conference, Florida State University, Tallahassee, Florida, March 14-16, 1985:
   R.B. King, "Dimensional and Topological Ideas Resulting from Consideration of Chemical Bonding in Polyhedral Cluster Compounds: The Concepts of Chemical Bonding Manifolds and Chemical Homeomorphism."

4. Mathematical Chemistry Workshop, Department of Mathematics, Florida State University, March 18, 1985:
   D.H. Rouvray, "Topological Indices as Chemical Behavior Descriptors."
   R.B.King, "Chirality Algebra."

5. Conference on Chemical Application of Graph Theory and Topology, University of South Carolina, Columbia, South Carolina, March 25-26, 1985:
   D.H. Rouvray, "Some New Uses of the Distance Matrix in Chemistry."
   R.B. King, "Graph Theoretical and Topological Ideas in the Structure and and Bonding in Polyhedral Cluster Compounds."

6. Conference on Graph Theory in Chemistry, Rutgers Center for Operations Research, Rutgers University, New Brunswick, New Jersey, June 15, 1985:
   D.H. Rouvray, "The Role of Topological Indices in Chemistry."

7. International Conference on Applications of Mathematical Concepts to Chemistry, Dubrovnik, Croatia, Yugoslavia, September 2-5, 1985:
   R.B. King, "Metal Cluster Topology: Applications to Gold and Platinum Clusters."
   D.H. Rouvray, "The Role of the Topological Distance Matrix in Chemistry."

8. SESAP Meetings of the American Physical Society, Athens, Georgia, December 2-4, 1985:
   M.H. Lee, "Dynamics of a Tagged Spin in the One-Dimensional Spin-=XY and Transverse Ising Model."

9. Dynamics Days, Fifth Annual Informal Workshop, Shelter Island, San Diego, California, January 7-10, 1986:
   R.B. King, "Systematics of Strongly Self-Dominant Higher Order Differential Equations Based on the Painlevé Analysis of Their Singularities."

10. Seventeenth Southeastern International Conference on Combinatorics, Graph Theory, and Computing, Florida Atlantic University, Boca Raton, Florida, February 10-14, 1986:
    D.H. Rouvray, "An Introduction to the Chemical Application of Graph Theory."
    D.H. Rouvray, "The Role of Graph-Theoretical Invariants in Chemistry."

11. Sanibel Symposium on Quantum Chemistry, Solid-State Theory, Many-Body Phenomena, and Computational Quantum Chemistry, Marineland, St. Augustine, Florida, March 10-15, 1986:
    R.B. King, "Graph Theory in the Study of Metal Cluster Bonding Topology: Applications to Metal Clusters Having Fused Polyhedra."

12. New York Academy of Sciences Conference on Perspectives in Biological Dynamics and Theoretical Medicine, Bethesda, Maryland, April 9-11, 1986:
    R.B. King, "Kinetic Logic as a Qualitative Approach for the Study of Oscillating and Chaotic Systems."

13. Society for Industrial and Applied Mathematics Third Conference on Discrete Mathematics, Clemson University, Clemson, South Carolina, May 14-16, 1986:
    R.B. King, "Directed Graphs in Dynamic Systems."
    D.H. Rouvray, "Characterization of Molecular Branching Using Topological Indices."
    E.R. Canfield, "P-Recursive Sequences."

14. Informal Minisymposium on Chemical Applications of Topology and Graph Theory, University of Georgia, Athens, Georgia, May 17, 1986:
    D.H. Rouvray, "The Topological Distance Matrix and Branching."
    M.P. Hanson, "Use of Topological Indices to Estimate the Sooting Tendencies of Hydrocarbon Fuels."
    C. Raychaudhury, "Topological Indices Characterizing Chemical Structure."
    R.B. King, "Polyhedral Rearrangements."

15. International Symposium on Computational and Mathematical Chemistry at the Sixty-Ninth Canadian Chemical Conference, University of Saskatchewan, Saskatoon, Saskatchewan, Canada, June 1-4, 1986:
    D.H. Rouvray, "The Modeling of Chemical Phenomena Using Topological Indices."
    R.B. King, "Polyhedra in Chemical Systems."

16. Sixteenth International Conference on Statistical Physics, Boston, Massachusetts, August 8-13, 1986:
    M.H. Lee and J. Hong, "Exact Dynamic Response and Local Field Corrections."
    N.L. Sharma and M.H. Lee, "Wavevector Dependent Susceptibility of a Free Electron Gas in D Dimensions."

17. Twenty-Fourth International Conference on Coordination Chemistry, University of Athens, Athens, Greece, August 24-29, 1986:
    R.B. King, "Mathematical Methods in Coordination Chemistry: Topological and Graph-Theoretical Ideas in the Study of Metal Clusters and Polyhedral Isomerizations."

18. International Symposium on the Physics and Chemistry of Small Clusters, Richmond, Virginia, October 28 - November 1, 1986:
    R.B. King, "Graph Theory Derived Methods for the Study of Metal Cluster Bonding Topology: Applications to Post-Transition Metal Clusters."

19. Conference on Graph Theory and Topology in Chemistry, University of Georgia, Athens, Georgia, March 15-20, 1987:
    M. Randić, V. Katović, D.J. Klein, W. Seitz, D.O. Oakland, and A.T. Balaban, "On Symmetry Properties of Chemical Graphs: Rearrangement of Axially Distorted Octahedra."
    S. El-Basil, "On Data Reduction of Chemical Information."
    M.P. Hanson and D.H. Rouvray, "The Use of Topological Indices to Estimate Melting Points of Organic Molecules."
    D.H. Rouvray, "The Fractal Nature of Alkane Physicochemical Behavior."
    R.B. King, "Topological Aspects of Infinite Metal Clusters and Superconductors."
    M.H. Lee, "Thermodynamics of Phase Transitions in Metal Cluster Systems."

20. March Meeting of the American Physical Society, New York, New York, March 16-20, 1987:
    M.H. Lee, "Langevin Analysis of the 1D Spin ½ XY and Traverse Ising Models."

21. Meeting of the European Physical Society, Pisa, Italy, April 5-8, 1987:
    M.H. Lee, "Method of Recurrence Relations and Applications to Many-Body Problems."

22. Workshop on Theoretical Immunology, Santa Fe, New Mexico, June 10-12, 1987:
    R.B. King, "Topological Aspects of Immunological Control Networks."

23. Topics in Chemical Physics and Related Areas, Zagreb, Yugoslavia, June 16-17, 1987:
    M. Randić, "Topics in Chemical Graph Theory."

24. International Course and Conference on the Interface Between Mathematics, Chemistry, and Computer Science, Dubrovnik, Yugoslavia, June 22-26, 1987:
    M. Randić, "On Symmetry of Graphs."
    M. Randić, "Molecular Topographic Descriptors."

25. 1987 Biennial Inorganic Chemistry Symposium: "Molecular Design of Materials: Applications of Mechanistic and Structural Organometallic Chemistry," Harvard University, Cambridge, Massachusetts, July 8-10, 1987:
    R.B. King, "Some Topological Aspects of Superconductivity in Inorganic Materials."

26. Sixth International Conference on Mathematical Modeling, St. Louis, Missouri, August 4-7, 1987:
    D.H. Rouvray, "The Search for Structural Requirements Determining the Mutagenicity of Nitrobenzenoid Compounds."
    M. Randić, S. El-Basil, and R.B. King, "On Non-Symmetry Equivalence."

27. Conference on Optoelectronics and Laser Applications in Science and Engineering, Los Angeles, California, January 10-17, 1988:
    M.H. Lee, "Electron Beam Propagation in Inhomogeneous Media."

28. Third University of California Conference on Statistical Mechanics, Davis, California, March 27-30, 1988:
    J. Florencio and M.H. Lee, "Memory Function and Relaxation Function of Some Spin Systems.

29. International Conference on the First Two Years of High Temperature Superconductivity, Tuscaloosa, Alabama, April 11-13, 1988:
    R.B. King, "Chemical Bonding Topology of Superconductors."

30. Annual Meeting of the Korean Physical Society, Seoul, Korea, April 23-24, 1988:
    M.H. Lee, "Method of Recurrence Relations."
    M.H. Lee, "Time Evolution in a Quantum System."

31. Third Chemical Congress of North America, Toronto, Ontario, Canada, June 5-10, 1988:
    R.B. King, "Graph Theory in the Study of Metal Cluster Bonding Topology: Application to Cobalt Carbonyl Carbide Clusters," paper INOR 232 in abstracts.

32. Third International Conference on the Interface Among Chemists, Mathematicians, and Computer Scientists, Dubrovnik, Yugoslavia, June 20-25, 1988:
    M.H. Lee, "Method of Recurrence Relations."
    M.H. Lee, "Applications to Time Evolutions."

33. Conference on Combinatorics of Symmetric Groups, Classical Algebra, and Special Functions, Oberwolfach, West Germany, July 3-9, 1988:
    E.R. Canfield, "The Use of Elliptic Functions in Solving Quintics."

34. Thirteen International Conference on Organometallic Chemistry, Torino, Italy, September 4-9, 1988:
    R.B. King, "The Seven Topologically Distinct Six-Vertex Polyhedra in Metal Carbonyl Cluster Chemistry," abstracts, p. 349.

35. Fourth European Symposium on Inorganic Chemistry, Freiburg, West Germany, September 12-15, 1988:
    R.B. King, "Topological Aspects of Metal Carbonyl Clusters with Alkylphosphinidene Vertices," paper A14 in abstracts.

36. 196th National Meeting of the American Chemical Society, Los Angeles, California, September 25-30, 1988:
    a. Symposium on the Physical Chemistry of High-Temperature Superconductors:
       R.B. King, "Chemical Bonding Topology of Superconductors," paper PHYS 9 in abstracts.
    b. Symposium on Computer Based Methods of Molecular Similarity:
       D.H. Rouvray, "The Evolution of the Concept of Molecular Similarity," paper COMP 42 in abstracts.

CUMULATIVE LIST OF PERSONNEL AT THE UNIVERSITY OF GEORGIA SUPPORTED BY THIS PROJECT

1. Dr. R. Bruce King, Regents' Professor of Chemistry and Principal Investigator
   May 15, 1984 to September 30, 1988.

2. Dr. M. Howard Lee, Professor of Physics
   February 15, 1985 to September 30, 1988.

3. Dr. E. Rodney Canfield, Professor of Computer Science
   May 15, 1984 to September 30, 1988.

4. Dr. Dennis H. Rouvray, Associate Research Scientist (Chemistry)
   September 1, 1984 to September 30, 1988.

5. Ms. Collette Pirie, Instructor of Computer Science
   May 15, 1984 to June 30, 1987.

6. Dr. Walapa Jatong, Post-Doctoral Fellow (Chemistry)
   August 1, 1985 to February 28, 1986.

7. Dr. Chandan Raychaudhury, Post-Doctoral Fellow (Chemistry)
   October 1, 1985 to August 31, 1986.

8. Dr. Milton Hanson, Professor Chemistry, Augustana College, Sioux Falls, South Dakota, on leave
   September 1, 1985 to May 31, 1986

9. Dr. Sherif El-Basil, Professor of Chemistry, University of Cairo, Egypt, on leave
   September 1, 1986 to September 30, 1987.

10. Dr. Milan Randić, Centennial Professor of Mathematics, Drake University, Des Moines, Iowa, on leave
    March 1, 1987 to August 31, 1987.

11. Dr. William L. Wilson, Post-Doctoral Fellow (Chemistry)
    November 1, 1984 to July 31, 1986.

12. Dr. Narayan Das Sadanani, Post-Doctoral Fellow (Chemistry)
    April 1, 1986 to December 31, 1986.

13. Dr. Gayatri Chorghade, Post-Doctoral Fellow (Chemistry)
    October 1, 1987 to August 31, 1988.

14. Dr. Nripendra Bhattacharyya, Post-Doctoral Fellow (Chemistry)
    January 1, 1988 to September 30, 1988.

15. Dr. João Florencio, Post-Doctoral Fellow (Physics)
    February 15, 1985 to August 31, 1987.

16. Dr. Natthi Lal Sharma, Post-Doctoral Fellow (Physics)
February 15, 1985 to December 31, 1985.

17. Dr. Elena Sevilla, Post-Doctoral Fellow (Physics)
September 1, 1987 to September 30, 1988

18. Dr. Ming Yu, Post-Doctoral Fellow (Physics)
June 1, 1988 to September 30, 1988.

19. Dr. Jonghae Hong, Assistant Professor of Physics, Seoul National University, Korea, on leave
January 1, 1985 to March 31, 1985; January 1, 1986 to March 31, 1986; July 1, 1986 to June 30, 1987; February 1, 1988 to February 29, 1988; June 1, 1988 to September 30, 1988.

20. Mr. Latif Khalil, Assistant Professor of Mathematics and Computer Science, St. Andrews Presbyterian College, Laurinburg, North Carolina, on leave
January 1, 1987 to June 30, 1987; June 1, 1988 to August 31, 1988.

21. Ms. Hitomi Kumazaki, Graduate Student (Chemistry)
January 1, 1988 to September 30, 1988.

22. Mr. Angus Laurie, Graduate Student (Chemistry)
April 1, 1988 to September 30, 1988

23. Mr. Jon Nelson, Graduate Student (Physics)
June 1, 1986 to December 31, 1986.

24. Mr. Surajit Sen, Graduate Student (Physics)
October 1, 1986 to September 30, 1988.

25. Mr. Ming Long, Graduate Student (Physics)
July 1, 1988 to September 30, 1988.

26. Mr. John Teel, Graduate Student (Computer Science)
October 1, 1984 to June 30, 1985.

27. Ms. Alison Nicklin, Undergraduate Scholar (Chemistry)
June 15, 1988 to August 15, 1988.

DEGREES GRANTED TO PERSONS WORKING ON THIS PROJECT

1. Mr. John Teel, Masters of Applied Mathematical Science, 1985.

2. Mr. Latif Khalil, Masters of Applied Mathematical Science, 1987.